

Non-ergodic dynamics of the extended anisotropic Heisenberg chain

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The issue of ergodicity is often underestimated. The presence of zero-frequency excitations in bosonic Green's functions determine the appearance of zero-frequency momentum-dependent quantities in correlation functions. The implicit dependence of matrix elements make such quantities also relevant in the computation of susceptibilities. Consequently, the correct determination of these quantities is of great relevance and the well-established practice of fixing them by assuming the ergodicity of the dynamics is quite questionable as it is not justifiable a priori by no means. In this manuscript, we have investigated the ergodicity of the dynamics of the z -component of the spin in the 1D Heisenberg model with anisotropic nearest-neighbor and isotropic next-nearest-neighbor interactions. We have obtained the zero-temperature phase diagram in the thermodynamic limit by extrapolating Exact and Lanczos diagonalization results computed on chains with sizes $L = 6 \div 26$. Two distinct non-ergodic regions have been found: one for $J'/J_z \lesssim 0.3$ and $|J_\perp|/J_z < 1$ and another for $J'/J_z \lesssim 0.25$ and $|J_\perp|/J_z = 1$. On the contrary, finite-size scaling of $T \neq 0$ results, obtained by means of Exact diagonalization on chains with sizes $L = 4 \div 18$, indicates an ergodic behavior of dynamics in the whole range of parameters.

I. INTRODUCTION

In order to study a physical system (i.e., to analyze its properties and its responses to external perturbations), we have to compute correlation functions C and susceptibilities χ (retarded Green's functions) of any operator ψ relevant to the dynamics under investigation

$$C(i, j) = \langle \psi(i) \psi^\dagger(j) \rangle \quad (1.1)$$

$$\chi(i, j) = -i\theta(t_i - t_j) \langle [\psi(i), \psi^\dagger(j)] \rangle, \quad (1.2)$$

where $\langle \dots \rangle$ stands for the average in some statistical ensemble, $i = (\mathbf{i}, t)$ for both spatial \mathbf{i} and temporal t coordinates. The operator ψ is taken in the Heisenberg picture.

In principle, one can compute the complete set of eigenstates $|n\rangle$ and eigenvalues E_n of the Hamiltonian describing the system under study. This knowledge makes possible to compute the Fourier transform in frequency of any correlation function as follows

$$C(\mathbf{i}, \mathbf{j}, \omega) = 2\pi\delta(\omega)\Gamma(\mathbf{i}, \mathbf{j}) + \frac{2\pi}{Z} \sum_{\substack{n, m \\ E_n \neq E_m}} e^{-\beta E_n} \langle n | \psi(\mathbf{i}) | m \rangle \langle m | \psi^\dagger(\mathbf{j}) | n \rangle \delta[\omega + (E_n - E_m)]$$

where the *zero-frequency function* $\Gamma(\mathbf{i}, \mathbf{j})$ is defined as^{1,2}

$$\Gamma(\mathbf{i}, \mathbf{j}) = \frac{1}{Z} \sum_{\substack{n, m \\ E_n = E_m}} e^{-\beta E_n} \langle n | \psi(\mathbf{i}) | m \rangle \langle m | \psi^\dagger(\mathbf{j}) | n \rangle. \quad (1.3)$$

Γ explicitly appears in the expression of the correlation function when the field ψ is boson-like, that is, ψ is constituted of an even number of original electronic (i.e., fermionic) operators^{1,2}. Hereafter, we focus on such a case.

According to the well-known relations existing between casual (C), retarded (R) Green's functions and correlation functions

$$\Re[G^R(\mathbf{k}, \omega)] = \Re[G^C(\mathbf{k}, \omega)] \quad (1.4)$$

$$\Im[G^R(\mathbf{k}, \omega)] = \tanh\left(\frac{\beta\omega}{2}\right) \Im[G^C(\mathbf{k}, \omega)] \quad (1.5)$$

$$C(\mathbf{k}, \omega) = -\left[1 + \tanh\left(\frac{\beta\omega}{2}\right)\right] \Im[G^C(\mathbf{k}, \omega)] \quad (1.6)$$

the zero-frequency excitations do not contribute explicitly to the imaginary part of the retarded Green's functions and, consequently, Γ does not explicitly appear in the expressions of susceptibilities. At any rate, susceptibilities retain an implicit dependence on Γ through the matrix elements $\langle n | \psi(\mathbf{i}) | m \rangle$. Then, the right procedure to compute both correlation functions and susceptibilities is clearly the one that starts from the causal Green's function, which is the only Green's function that explicitly depends on Γ .

It is worth noticing that the value of Γ dramatically affects the values of directly measurable quantities (e.g., compressibility, specific heat, magnetic susceptibility, ...) through the values of correlation functions and susceptibilities. According to this, whenever it is possible, Γ should be exactly calculated case by case.

If we do not have access to the complete set of eigenstates and eigenvalues of the system, which is the rule in the most interesting cases, we have to compute correlation functions and susceptibilities within some, often approximated, analytical framework. Now, since no analytical tool can easily determine Γ (e.g., the equations of motion cannot be used to fix Γ as it is constant in time), one usually assumes the ergodicity of the dynamics of ψ and simply substitutes Γ by its ergodic value:

$$\Gamma^{erg}(\mathbf{i}, \mathbf{j}) = \langle \psi(\mathbf{i}) \rangle \langle \psi^\dagger(\mathbf{j}) \rangle. \quad (1.7)$$

Unfortunately, this procedure cannot be justified a priori

(i.e., without computing Γ through its definition (1.3)) by absolutely no means. The existence of just one integral of motion divides the phase space into separate subspaces not connected by the dynamics. This latter, in turn, becomes non ergodic: time averages give different results with respect to ensemble averages.

The lack of ergodicity has sizable effects. One of its manifestations is the well-known difference between the static isolated (or Kubo) susceptibility and the isothermal one³. The dynamics of an operator ψ , in a system described by the Hamiltonian H , is said to be ergodic if³

$$\lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle \psi \psi^\dagger(t) \rangle dt = \langle \psi \rangle \langle \psi^\dagger \rangle, \quad (1.8)$$

where $\langle \dots \rangle$ stands, for instance, for the canonical average at temperature T

$$\langle \psi \rangle = \frac{1}{Z} \text{Tr}(\psi e^{-\beta H}), \quad (1.9)$$

with $\beta = \frac{1}{T}$ and $Z = \text{Tr}(e^{-\beta H})$. That is, the dynamics of ψ is ergodic if, during its time evolution, it has non-zero matrix elements only between states within a zero-volume region of the phase space of the system. Only in this case, the equilibrium averages (l.h.s. of (1.8)) are equal to the ensemble averages (r.h.s. of (1.8)), which are much easier to compute. Now, one can show⁴ that the difference between the static (or Kubo) susceptibility

$$\begin{aligned} \chi(0) &= \lim_{\omega \rightarrow 0} \mathcal{F}[-i\theta(t)\langle [\psi, \psi^\dagger(t)] \rangle] \\ &= \int_0^\beta \langle \psi \psi^\dagger(i\lambda) \rangle d\lambda - \beta \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle \psi \psi^\dagger(t) \rangle dt, \end{aligned} \quad (1.10)$$

and the isothermal susceptibility

$$\chi^T = \left. \frac{\delta \langle \psi \rangle}{\delta \mathcal{H}} \right|_{\mathcal{H} \rightarrow 0} = \int_0^\beta \langle \psi \psi^\dagger(i\lambda) \rangle d\lambda - \beta \langle \psi \rangle \langle \psi^\dagger \rangle, \quad (1.11)$$

is just proportional to the difference between the l.h.s. and the r.h.s. of (1.8)

$$\chi^T - \chi(0) = \beta \left(\lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle \psi \psi^\dagger(t) \rangle dt - \langle \psi \rangle \langle \psi^\dagger \rangle \right). \quad (1.12)$$

In the above, \mathcal{F} stands for the Fourier transform and \mathcal{H} for the external field coupled to ψ (e.g., an external magnetic field in the case of magnetization). The second line of (1.10) comes from the relation between susceptibility and relaxation function. Γ (as defined in (1.3)) is exactly equal to the l.h.s. of (1.8).

Thus, it is clear that issue of ergodicity is relevant to linear response too. It is also worth noting that non-ergodicity at zero temperature is just the result of a degeneracy in the ground state, which would be lifted by

a vanishing ψ - \mathcal{H} coupling in the Hamiltonian. For instance, the reader can imagine a ferromagnetic ground state with finite spontaneous magnetization driven by a vanishing external magnetic field.

Many systems exhibit non-ergodic dynamics. Over the last years, we have been studying^{1,5} some of them analytically by means of the Composite Operator Method^{1,2}: two-site Hubbard model, three-site Heisenberg model, tight-binding model in magnetic field, double-exchange model, extended Hubbard model in the ionic limit. Recently, we have started an investigation of such models also by means of numerical techniques: Lanczos and Exact Diagonalization. Along this latter line, in the present paper, we calculate Γ for the z -component of the spin at site \mathbf{i} , $S_{\mathbf{i}}^z$, in the one-dimensional anisotropic extended Heisenberg model (see next section) and show that it takes non-ergodic values in some regions of the parameter space of the model both for finite sizes and in the bulk limit. This analysis is the natural continuation of that reported in Ref. 6, where we have analyzed the standard (isotropic and non-extended) Heisenberg model at zero temperature and found a non-ergodic behavior of Γ .

II. DEFINITIONS AND METHOD

We have studied the ergodicity of dynamics of the operator $S_{\mathbf{i}}^z$ in the 1D anisotropic extended Heisenberg model described by the following Hamiltonian:

$$\begin{aligned} H &= -J_z \sum_{\mathbf{i}} S_{\mathbf{i}}^z S_{\mathbf{i}+1}^z \\ &+ J_\perp \sum_{\mathbf{i}} (S_{\mathbf{i}}^x S_{\mathbf{i}+1}^x + S_{\mathbf{i}}^y S_{\mathbf{i}+1}^y) + J' \sum_{\mathbf{i}} \mathbf{S}_{\mathbf{i}} \mathbf{S}_{\mathbf{i}+2}, \end{aligned} \quad (2.1)$$

where $S_{\mathbf{i}}^x$, $S_{\mathbf{i}}^y$ and $S_{\mathbf{i}}^z$ are the x , y and z components of the spin-1/2 at site \mathbf{i} , respectively. The model (2.1) is taken on a linear chain with periodic boundary conditions. We take the interaction term parameterized with J_z ferromagnetic ($J_z > 0$) and the next-nearest-neighbor interaction term, which is parameterized with J' , isotropic. In order to frustrate ferromagnetism, we have considered only the case with $J' > 0$, that is, with an antiferromagnetic coupling between next-nearest neighbors. According to this, only chains with even number of sites have been studied in order to avoid topological frustration that would be absent in the thermodynamic limit. Since it is possible to exactly map all results obtained for $J_\perp > 0$ to those for $J_\perp < 0$ by means of a simple canonical transformation, we have limited our study only to positive values of J_\perp .

We have found some numerical^{7,8,9,10,11} and few analytical studies^{12,13} of the model (2.1) in the literature, mainly in the antiferromagnetic state ($J_z < 0$). Only one fixed point ($J_\perp = J_z$ and $J' = J_z/2$) is known to possess an analytic ground state¹⁴. In the rest of the phase diagram, the model (2.1) seems not to be integrable^{15,16}.

We have numerically diagonalized the Hamiltonian (2.1) for chains of size L ranging between 6 and 18 by means of Exact Diagonalization (ED) (divide and conquer algorithm) and for chains of size L ranging between 20 and 26 by means of Lanczos Diagonalization (LD). We have systematically taken into account translational symmetry and classified the eigenstates by the average value of $S^z = \sum_i S_i^z$, which is a conserved quantity. Whenever we have used ED, all eigenvalues and eigenvectors of (2.1) have been calculated up to machine precision and, therefore, we have been able to determine the exact dynamics of the system for all temperatures. On the contrary, when we have used LD, we have been limited to the zero-temperature case since only the ground state can be considered exact in LD.

As already discussed above, the dynamics of an operator (e.g., S_i^z) is ergodic whenever (1.8) is satisfied, or equivalently, (1.3) is equal to its *ergodic* value:

$$\Gamma^{erg} = \langle S_i^z \rangle^2 = \frac{1}{Z^2} \sum_{n,m} e^{-\beta(E_n + E_m)} \langle n | S_i^z | n \rangle \langle m | S_i^z | m \rangle. \quad (2.2)$$

The dynamics of a finite system is hardly ergodic, since (1.3) and (2.2) unlikely coincide. In the thermodynamic limit, the sums in (1.3) and (2.2) become series and no conclusion can be drawn *a priori*. Since we have diagonalized the Hamiltonian (2.1) numerically (i.e., only for finite systems) and since $L \rightarrow \infty$ is the most interesting case, we have analyzed our results through finite-size scaling in order to speculate on the properties of the bulk system.

III. ZERO-TEMPERATURE RESULTS

If the ground state of (2.1) is N -fold degenerate then, at $T = 0$, (1.3) and (2.2) read as follows:

$$\Gamma = \frac{1}{N} \sum_{n,m=1}^N |\langle n | S_i^z | m \rangle|^2$$

$$\Gamma^{erg} = \left(\frac{1}{N} \sum_n \langle n | S_i^z | n \rangle \right)^2,$$

respectively.

Thanks to the translational invariance enjoined by the system $\langle S_i^z \rangle$ is independent of i and proportional to the z -component of the total spin operator average $\langle S_{tot}^z \rangle$. It is easy to show that, even if there is a finite magnetic moment per site in any of such N degenerate ground states, $\langle S_i^z \rangle$ at $T = 0$ is always zero in absence of magnetic field. Indeed, if a ground state with non-zero $\langle S_i^z \rangle = M$ exists, also another ground state with $\langle S_i^z \rangle = -M$ exists. Thus, at zero temperature, Γ^{erg} is always zero and the only quantity of interest is Γ . A finite value of this latter implies non-ergodicity. Obviously, if $N = 1$ then both values coincide. Therefore, a non-ergodic phase corresponds to degenerate ground states with finite magnetization.

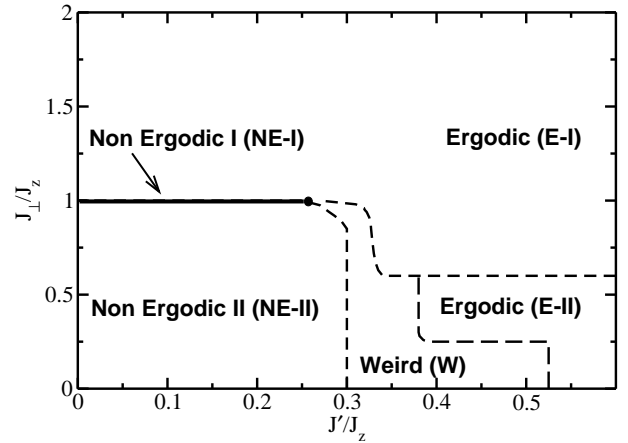


FIG. 1: Zero-temperature ergodicity phase diagram in the $J' - J_\perp$ plane. Due to the symmetry of the Hamiltonian only the upper half is shown (see in the text). Only two ergodic phases (E-I and E-II) have been found in the reported parameter space. The others are either non-ergodic (NE-I and NE-II) or impossible to conclusively analyze (W). The latter phase might shrink to a transition line in the bulk limit.

In the studied range of coupling constants (see Fig. 1) we have found two non-ergodic phases (NE-I and NE-II), two ergodic ones (E-I and E-II) and a *weird* phase (W). Our computational facilities limit the range of chain sizes that we can analyze such that we could not establish, by means of finite-size scaling, whether the *weird* phase (W) is ergodic or not. In the non-ergodic phases (NE-I and NE-II), we were able not only to perform the finite-size scaling, but also to write down an analytic expression for Γ as a function of the chain size L . The *weird* phase (W) has exhibited a strong dependence of the ground state upon the particular values of the couplings. On the contrary, the other phases exhibit ground states that are independent of the particular values of the coupling constants.

Ergodicity of the standard Heisenberg model ($J' = 0$ and $J_\perp = J_z$) at $T = 0$ has already been studied in Ref. 6: the dynamics is non-ergodic for ferromagnetic coupling ($J_\perp = J_z < 0$) as the system has a $L + 1$ degenerate ground state

$$\Gamma = \frac{1}{12} + \frac{1}{6L}. \quad (3.1)$$

It is clear from (3.1) that Γ remains non-ergodic also in the thermodynamic limit. This point ($J' = 0$ and $J_\perp = J_z$) becomes a line in our phase diagram and is denoted as NE-I (see Fig. 1). In fact, the next-nearest-neighbor interaction J' may frustrate ($J' > 0$) or favor ($J' < 0$) the ferromagnetism. In the latter case, the ground state remains unchanged for any value of $J' < 0$. Therefore, we expect the line denoting the phase NE-I to extend also to negative J' . If, on the contrary, J' is positive and large enough to frustrate the system in such a way that the ground state loses its ferromagnetic character, the ergodicity is restored. This occurs at a

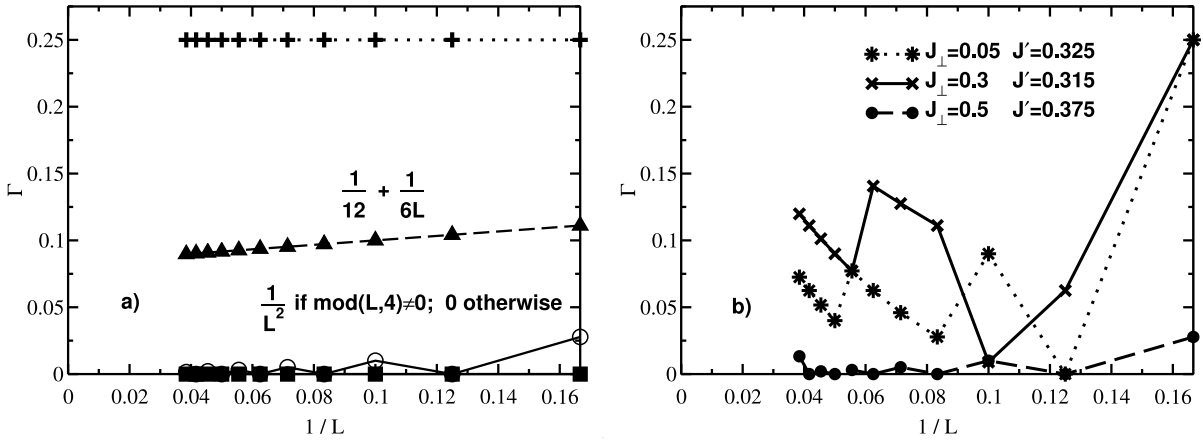


FIG. 2: Finite-size scaling in the case of $T = 0$ for different points in the phase diagram of Fig. 1. Symbols on panel a): + corresponds to (NE-II), \blacktriangle corresponds to (NE-I), \blacksquare corresponds to (E-I) and \circ to (E-II) regions of Fig. 1, respectively. On panel b) different examples from (W) region are shown. Hamiltonian couplings are shown in the legend. All energies are expressed in units of J_z .

finite critical $J' \sim 0.25J_z$. For values of J' larger than the critical one, we find a non-degenerate ground state with $\langle S_{tot}^z \rangle = 0$.

If $J_{\perp} \neq J_z$ the rotational invariance is broken so that states with the same $\langle \mathbf{S}_{tot}^2 \rangle$, but different $\langle S_{tot}^z \rangle$, are not degenerate anymore. In the non-ergodic region (NE-II) of the phase diagram (see Fig. 1), the ground state is just doubly degenerate (not $L + 1$ degenerate as in (NE-I)): one ground state corresponds to a configuration with all spins *up* and the other to a configuration with all spins *down*. Hence, the value of Γ in this phase is $1/4$ and does not depend neither on the Hamiltonian couplings nor on the number of sites in the chain. It is clear that also this phase extends to negative values of J' . This kind of ground state stands the frustration introduced by next-nearest-neighbor interaction up to $J' \sim 0.3J_z$ (see Fig. 1).

The ergodic region (E-I) of the phase diagram (see Fig. 1) has $\Gamma = 0$ for all sizes of the system and values of the couplings: the unique ground state belongs to the sector with $\langle S_{tot}^z \rangle = 0$. On the contrary, the other ergodic phase (E-II) has non-zero values of Γ for values of L not multiples of four. The ground state in this phase has average total spin equal to one and, therefore, $\Gamma = 1/L^2$. We obviously conclude that (E-II) phase is ergodic in the thermodynamic limit.

The values of Γ in these four phases (NE-I, NE-II, E-I and E-II) exhibit perfect finite-size scaling as shown in Fig. 2a). This has allowed us to make definite statements also in the thermodynamic limit.

The *weird* phase (W) (see Fig. 1) is characterized by a quite strong size dependence, as shown in Fig. 2b) where a tentative finite-size scaling of Γ in the different points of the phase is presented. This region manifests a diverging finite-size scaling within the range of sizes we were able to handle. In this case, the behavior of Γ as a function of L strongly depends on the particular choice of

the Hamiltonian couplings and is highly non monotonous when increasing L , according to the strong dependence on L of $\langle S_{tot}^z \rangle$ in the ground state. In this critical region the eigenvalues of (2.1) present many level crossings, which means that the maximum value of L we were able to reach ($L_{max} = 26$) is not large enough to perform a sensible finite-size scaling analysis. However, we expect that this phase becomes ergodic in the thermodynamic limit, although still different from the ergodic phases E-I and E-II.

We can summarize our findings in the thermodynamic limit at zero temperature as follows:

$$\Gamma = \begin{cases} \frac{1}{12} & \text{if } J_{\perp} = \pm J_z \text{ and } J' \lesssim 0.25J_z \\ \frac{1}{4} & \text{if } |J_{\perp}| < J_z \text{ and } J' \lesssim 0.3J_z \\ ??? & \text{in the weird phase (W) (see Fig. 1)} \\ 0 & \text{otherwise} \end{cases} \quad (3.2)$$

IV. FINITE-TEMPERATURE RESULTS

At zero temperature, the degeneracy of the ground state is clearly the source of non-ergodicity. At finite temperatures, all states contribute to the dynamics of the system and we have to search for some other source of non-ergodicity, if any. In fact, when the sum in (1.3) becomes an integral, the degree of degeneracy of a state with energy ε is given by the value of the density of states at ε . Then, the result of the integration is hard to guess. Once again, we have used finite-size scaling in order to reveal the behavior in the bulk system. Ergodic value of Γ should now be calculated through the thermal average:

$$\Gamma^{erg} = \left(\frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | S_i^z | n \rangle \right)^2. \quad (4.1)$$

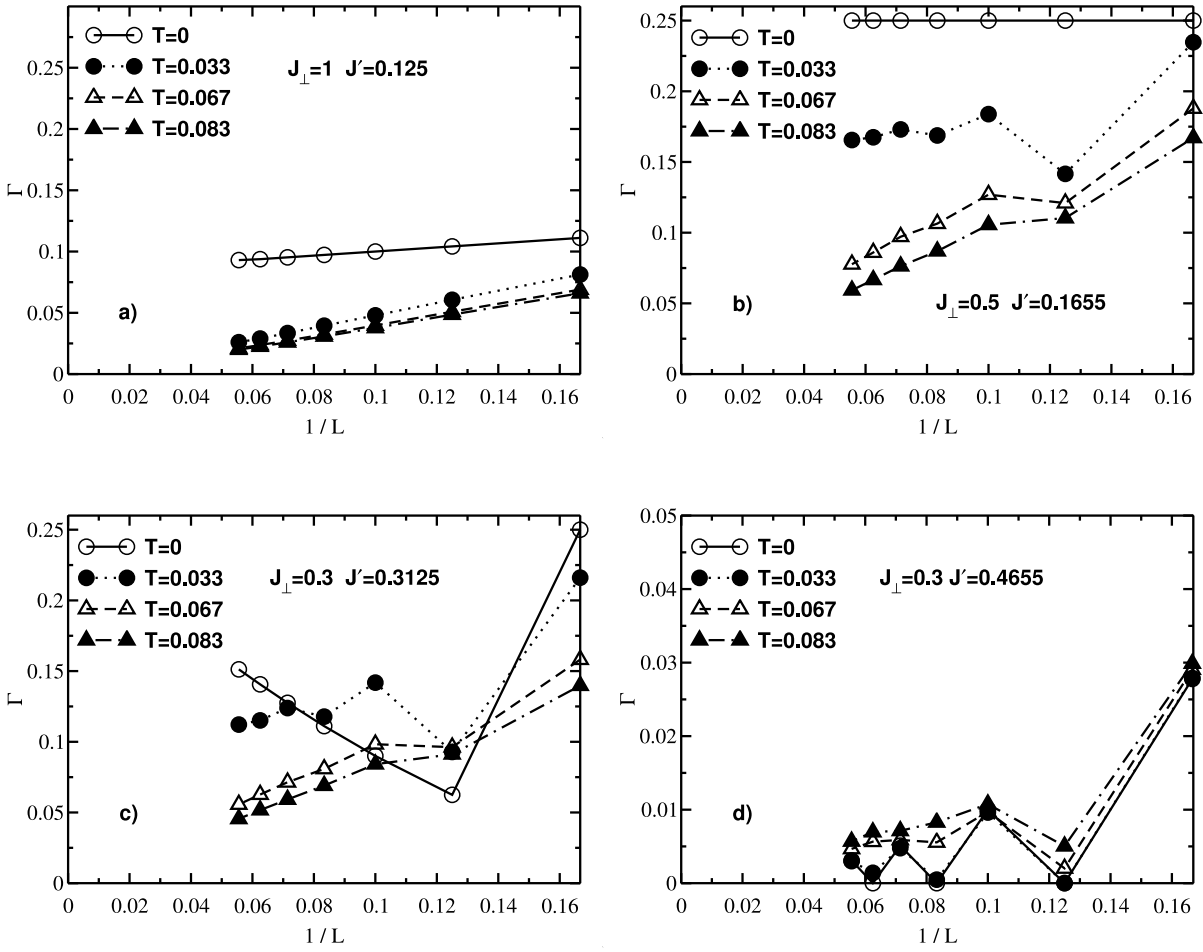


FIG. 3: Finite-size scaling of the finite-temperature results for different representative points on the phase diagram of Fig. 1. a) NE-I phase. b) NE-II phase. c), d) two sample points from the *weird* (W) phase, which at $T = 0$ show quite distinct finite-size scaling and at $T > 0$ behave very similarly. All energies are measured in units of J_z . All the data suggest that the bulk system at $T > 0$ is always ergodic.

It follows that Γ^{erg} is just zero for all Hamiltonian couplings.

We have computed finite-size scaling at several finite temperatures using ED. In Fig. 3, four representative points from the phase diagram in Fig. 1 are shown: the plots from panels a) and b) belong to the former NE-I and NE-II phases, while those from panels c) and d) belong to the W one. Finite-size scaling for the ergodic phases (E-I and E-II) gives Γ identically zero and is not reported. Already at low temperatures ($T \sim 0.08J_z$) and small sizes $L \leq 18$, our calculations show a very clear indication that, in the thermodynamic limit, Γ is zero in the whole phase diagram. In addition, we have found that Γ approaches zero nearly proportional to L^{-1} for finite systems.

These results can be analyzed from another point of view. As it is stated by Suzuki³, necessary and sufficient condition for the ergodicity of the dynamics of an operator A under the Hamiltonian H is the orthogonality of

A to all the integrals of motion of the system

$$(A, H^i) = 0, \quad (4.2)$$

where $\{H^i\}$ represents the complete set of integrals of motion of the Hamiltonian H . $\{H^i\}$ form a linear space with metrics given by the normalized density matrix

$$(H^i, H^j) = \frac{1}{Z} \sum_k e^{-\beta E_k} H_{k,k}^i H_{k,k}^j \equiv \langle H^i H^j \rangle, \quad (4.3)$$

where H^i and H^j are two integrals of motion and the sum is extended on all microscopic states of the system. Then, for a given operator A , to be orthogonal to all integrals of motion of H means either (i) to be off-diagonal with respect to H or (ii) to have a negligible number of diagonal matrix elements so that the scalar products (4.2) would go to zero in the thermodynamic limit. It follows that the dynamics of an integral of motion is surely non-ergodic, since it is surely not orthogonal to itself.

For finite systems, the response is practically always non-ergodic as it is unlikely that (1.3) is exactly zero. In

fact, for any fixed size, Γ is non zero (see Fig. 3). Naively, one could expect that S_i^z has non-ergodic dynamics also at finite temperatures since its average is proportional to the one of S_{tot}^z , which is an integral of motion. However, our numerical studies suggest that case (ii) applies to this operator. It is worth noticing that this type of behavior can be strongly dependent on the dimensionality of the system. For instance, we can expect a non-ergodic dynamics also at finite temperatures in higher dimensions, where a finite critical temperature for the transition to the ferromagnetic phase exists.

As it results from our analysis, the question of ergodicity of a spin system is closely connected to the presence of a finite magnetic moment per site. It might seem, therefore, that since we are dealing with a one-dimensional system, we could apply the Mermin-Wagner theorem¹⁷ and exclude the possibility to have finite magnetization at $T \neq 0$. Actually, our model is not isotropic so one of the conditions of Mermin-Wagner theorem is not met. At any rate, even along the line $J_\perp = J_z$ the proof of the above theorem involves the introduction of an infinitesimally small magnetic field that would split the degeneracy and make ergodic the system dynamics.

V. CONCLUSIONS

Summarizing, we have studied the 1D anisotropic Heisenberg model with next-nearest-neighbor exchange

interaction and the ergodicity of the operator S_i^z by means of the Lanczos and Exact Diagonalization techniques. At zero temperature, we have constructed the ergodicity phase diagram and found two distinct non-ergodic regions in the thermodynamic limit. The borders of these regions and the corresponding non-ergodic values of Γ have been determined by means of a finite-size scaling analysis of the Lanczos data. The results of this analysis (i.e., critical couplings and non-ergodic Γ values, see (3.2)) can be used by analytic methods that aim at computing physical properties and response functions of this system. Our results for finite temperatures suggest the ergodicity of the dynamics in the thermodynamic limit in the whole range of couplings. It implies, on the basis of Suzuki theorem³, that the number of diagonal matrix elements of S_i^z in the energy representation is negligible in the thermodynamic limit. A finite-size system, instead, remains non ergodic and the finite- L corrections to the bulk value of Γ are proportional to the inverse volume of the system (i.e., to L^{-1}).

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